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Molecular dynamics study of the structure and performance of simple and double bases propellants

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Abstract

To investigate the structure and performance of simple and double bases propellants, the nitrocellulose (NC), nitroglycerin (NG), and double mixed system (NC + NG) have been simulated by using the molecular dynamics (MD) method with the COMPASS force field. The interactions between NC and NG have been analyzed by means of pair correlation functions. The mechanical properties of the three model systems, i.e. elastic coefficients, modulus, Cauchy pressure, and Poisson's ratio, etc., have been obtained. It is found that the rigidity, ductibility, and tenacity of the double bases propellants (NC + NG) are stronger than those of simple base propellants (NC), which attributes to the effect of NG and the strong interactions between NC and NG. The detonation properties of the three systems have also been calculated and the results show that compared with the simple base propellant (NC), the detonation heat and detonation velocity of the double base propellants (NC + NG) are increased.

Keywords: Molecular dynamics (MD); Propellant; Mechanical property; Detonation property

1. Introduction

Propellant, known as a kind of energetic materials for launching, usually contains fuel and oxidizer components. It has widespread application in weapon equipment, space navigation, and industrial and agricultural production, so researches on propellant have received great attention for a long time. A typical simple base propellant consists of a simple compound, usually nitrocellulose (NC), and a double bases propellant usually consists of NC and nitroglycerin (NG), to which a plasticizer is added [1–4]. Both simple base and double bases propellants are homogeneous. Modern composite propellants are heterogeneous mixtures, which use a crystallized salt as an oxidizer and aluminum as fuel. For a composite propellant, the relationship between its formulation and performance plays a key role in its formulation design. Therefore, much experimental work has been done to investigate the issues related to the structure, formulation, and properties of propellants. Computer simulations have increasingly played an important role in this field. They can make it possible to screen candidate formulation designs, thereby avoiding expensive experimental tests. In addition, simulations may provide an understanding of the structure–performance relationships in propellants, which in turn can help design better and more efficient laboratory tests.

A force field method, especially molecular dynamics (MD) method, is an important and effective method to study the structure and performance of materials at present. Recently, our institute firstly utilizes MD method to study the polymer-bonded explosive (PBX), a composite material [5–12]. Yet there is no MD-based studies reported on this kind of propellant. In this study we choose simple and double bases propellants as an example to investigate the structure–performance relationships. The destination in this study is to test the force field, method, and model, and to understand the correlations between the structure and performance for propellants. It is hoped that our studies provide some information and guidance for composite formulation design.

2. Computational approach and details

2.1. Computational model

The initial models were built by using materials studio (MS) package [13]. As for NC, the backbone conformation is critical to

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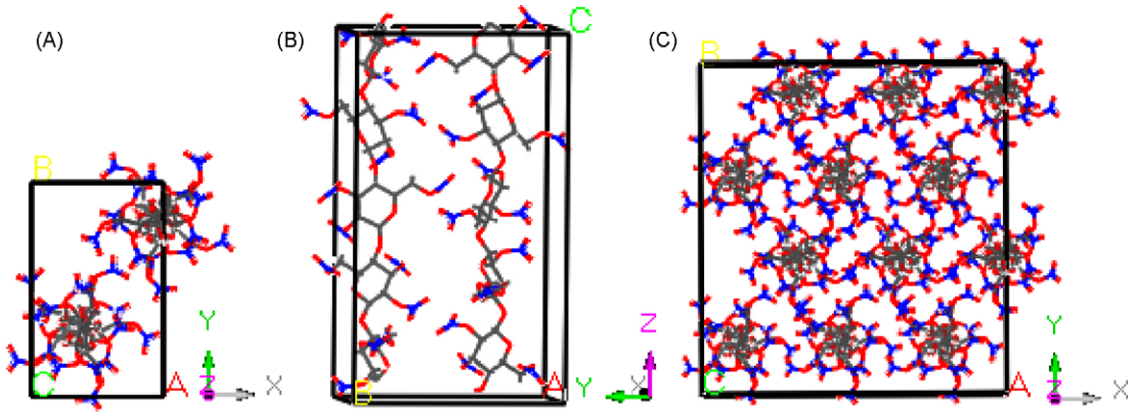

Fig. 1. The primitive cell of NC and its supercell (3 × 2 × 1) (C). (A) Top view, (B) side view and (C) initial model of simple base propellant.

its performance. Due to lacking of the whole bulk cell parameters and space group of NC, we built its molecular chain with 5_2 helix conformation suggested by Meader et al. [14]. Two chains of polymer NC were placed in a periodic box with the lattice vectors of $a = 0.90$ nm, $b = 1.46$ nm, and $c = 2.54$ nm, the lattice angles of $\alpha = \beta = \gamma = 90°$, and the density of 1.49 g cm^{-3}. Therefore, the primitive cell of NC was obtained (see Fig. 1A and B) and the initial model of simple base propellant was established and shown in Fig. 1C.

The initial β-nitroglycerin (NG) structure was built based on X-ray diffraction data [15], with four molecules in a cell and Fig. 2 shows its primitive cell and supercell. When the hydroxyl groups (–OH) of cellulose are replaced by nitro groups (–NO_2), the products are obtained with one, two or three substitutions and their nitrogen containing (N%) is 6.75, 11.11, and 14.14%, respectively. In fact, we always get their mixture with diverse substitution products due to difficulty in being nitrified completely. The simple base propellant with nitrogen containing of 13.0% or above, was built from cellulose trinitrate in order to simplify the model.

As for the double bases propellant with its nitrogen containing of 12.0%, we built the initial model as follows in order to meet the practical requirement of composite design. To emphasize the interaction between NC and NG, we choose the side of NC, not the end groups, to contact NG because of the nitro groups existing in outer side of the helix chain of NC. The double bases propellant model contains 10 helix NC chains and 43 NG molecules, with mass percentage of 58.1 and 41.9%, respectively, and is shown in Fig. 3.

Therefore, we get the three initial models for the MD simulations, as shown in Figs. 1C, 2B and 3.

2.2. MD simulations

The COMPASS force field [16] is used to study the structures and properties of the NC, NG, and NC + NG. Its parameters have been debugged and ascertained from the *ab initio* calculations, optimized according to the experimental values, and parameterized using extensive data for molecules in condensed phase. Its nonbonded parameters have been further amended and val-

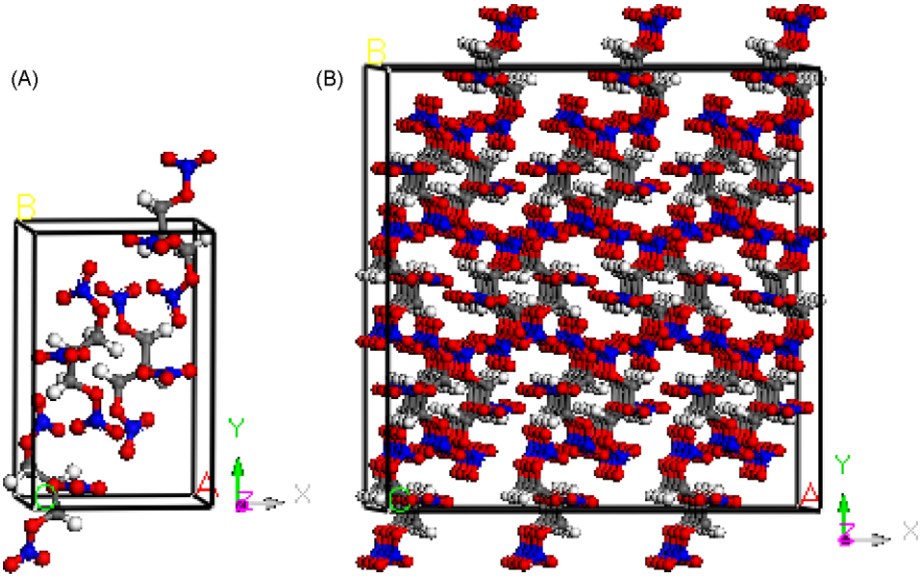

Fig. 2. The primitive cell and supercell of β-nitroglycerin (NG). (A) Primitive cell and (B) supercell (3 × 2 × 4) of NG.